International Journal of

Quantum Chemistry

Contents for Volume 69, 1998

Issue No. 1, 1998

Special Issue: Theoretical Chemistry in Biology: From Molecular Structure to Functional Mechanisms
Guest Editors: Peter Kollman and Harel Weinstein

Introduction
P. Kollman, H. Weinstein, and M. Zerner **1**

Toward a Charge-Transfer Model of Neuromolecular Computing
R. Wallace, H. Price, and F. Breitbeil **3**

Vanadate Complex Spectroscopy at the RNase A Active Site
M. Krauss and B. D. Wladkowski **11**

Development of Pharmacophores for Inhibitors of the Rapid Component of the Cardiac Delayed Rectifier Potassium Current
P. Mátyus, A. P. Borosy, A. Varró, J. G. Papp, D. Barlocco, and G. Cignarella **21**

A Comparative Study of O_2, CO, and NO Binding to Iron–Porphyrin
C. Rovira, K. Kunc, J. Hutter, P. Ballone, and M. Parrinello **31**

Ab Initio Study of the Structure of Isocytosine–Cytosine Standard Watson–Crick Base Pairs in the Gas Phase and in Water
N. U. Zhanpeisov and J. Leszczynski **37**

Correlation of Di- and Tripeptide Distribution Coefficients with Structure via Unitary Molecular Indices
S. P. Molnar and J. W. King **49**

Screened Coulomb Potential Based Implicit Solvent Model: Formulation and Parameter Development
F. Guarnieri, A. B. Schmidt, and E. L. Mehler **57**

Rational Design of a Targeted Combinatorial Chemical Library with Opiatelike Activity
W. Zheng, S. J. Cho, and A. Tropsha **65**

Calculation of Ligand Binding Free Energies from Molecular Dynamics Simulations
J. Marelius, T. Hansson, and J. Åqvist **77**

Ab Initio and Density Functional Theory Studies of the Catalytic Mechanism for Ester Hydrolysis in Serine Hydrolases
C.-H. Hu, T. Brinck, and K. Hult **89**

Bacteriorhodopsin α-Helices in Lipid Settings: Insights for Structure Prediction
T. B. Woolf **105**

Theoretical Study of Metiamide, A Histamine H_2 Antagonist
J. B. L. Martins, C. A. Taft, M. A. Perez, F. M. L. G. Stamato, and E. Longo **117**

List of Participants **129**

Call for Contributions **137**

Call for Contributions **139**

Call for Contributions **141**

Call for Contributions **143**

Issue No. 2, 1998

Theoretical and Computational Developments

Self-Consistent Thomas–Fermi–Dirac Theory, Extended by Gell-Mann and Brueckner Correlation, in Terms of Density n and Its Two Reduced Gradients $\nabla^2 n/n$ and $\nabla n/n$
N. H. March, A. Holas, and Á. Nagy **145**

Implementation of Gradient-Optimization Algorithms and Force Constant Computations in BSSE-Free Direct and Conventional SCF Approaches
A. Famulari, E. Gianinetti, M. Raimondi, and M. Sironi **151**

Extension of the Quantum Virial and Hellmann–Feynman Theorems to the Quantum Statistical Averages
D. Popov **159**

A Parallel Green's Operator for Multidimensional Quantum Scattering Calculations
Å. Edlund and U. Peskin **167**

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Second-Order Shakeup Terms in Electron Propagator Calculations on F_2 and H_2O_2
J. V. Ortiz **175**

Semiclassical Self-Consistent Field Perturbation Theory for the Hydrogen Atom in a Magnetic Field
A. V. Sergeev and D. Z. Goodson **183**

Electron Pairing and Chemical Bonds: Chemical Bonds from the Condition of Minimum Fluctuation of Electron Pair
R. Ponec **193**

Properties, Dynamics, and Electronic Structure of Condensed Systems and Clusters

Could Alkaline–Earth-Intercalated Fullerites Actually be Semimetals?
E. B. Starikov **201**

Three-Dimensional Crystal-Orbital Calculations on Crystallohydrates of Mononucleotide Salts. III. Valence-Split Basis Sets
E. B. Starikov **209**

Call for Contributions **219**

Call for Contributions **221**

Call for Contributions **223**

Call for Contributions **225**

Issue No. 3, 1998

Special Issue: Symposium on Density Functional Theory and Applications (Part I of II)
Guest Editors: Weitao Yang and Mel Levy
Special Editor: Sam Trickey

Introduction **227**

List of Participants **229**

How Robust is Present-Day DFT?
E. R. Davidson **241**

Optimized Potential Method for Ensembles of Excited States
Á. Nagy **247**

Theoretical Determination of Exact-Exchange-Mixing Parameter Employing the Ionization Energy Theorem
J. B. Krieger, J. Chen, and G. J. Iafrate **255**

Exact Exchange Kernel for Time-Dependent Density-Functional Theory
A. Görling **265**

Quantum Fluid Density Functional Theory of Time-Dependent Processes
P. K. Chattaraj, S. Sengupta, and A. Poddar **279**

Time-Dependent Density-Functional Theory with Optimized Effective Potential and Self-Interaction Correction: Application to the Study of Coherent Control of Multiple High-Order Harmonic Generation of He Atoms in Mixed Laser Fields
X.-M. Tong and S.-I Chu **293**

Generalized Floquet Theoretical Formulation of Time-Dependent Density Functional Theory for Many-Electron Systems in Multicolor Laser Fields
D. A. Telnov and S.-I Chu **305**

Quantum Chemical Molecular Dynamics
B. I. Dunlap **317**

The Application of Approximate Density Functionals to Complex Systems
O. F. Sankey, A. A. Demkov, W. Windl, J. H. Fritsch, J. P. Lewis, and M. Fuentes-Cabrera **327**

Mixed Lead–Alkali Clusters in the Gas Phase and in Liquid Alloys
L. M. Molina, M. J. López, A. Rubio, J. A. Alonso, and M. J. Stott **341**

Full-Potential Optical Calculations of Lead Chalcogenides
A. Delin, P. Ravindran, O. Eriksson, and J. M. Wills **349**

Exchange–Correlation Corrections to Lattice Dynamics of Simple Metals, and a Search for Soft Modes at Normal and Expanded Volume
L. Pollack and J. P. Perdew **359**

Theoretical Study of Transition-Element Carbonyls MCO and Carbenes MCH_2 (M = Ti, Fe, Ni) in the Ground and First Electronic Excited States by DFT Methods
R. M. Sosa, P. Gardiol, and G. Beltrame **371**

DFT Investigations of the Structure and Bonding Between Transition Metals and Olefins
H. Bögel, S. Tobisch, and T. Nowak **387**

Frozen Density Matrix Approach for Electronic Structure Calculations
T.-S. Lee and W. Yang **397**

Toward Linear Scaling with Fitted Exchange–Correlation Terms in the LCGTO-DF Method via a Divide-and-Conquer Approach
S. K. Goh, R. T. Gallant, and A. St-Amant **405**

A Scattering Theoretic Approach to Scalar Relativistic Corrections on Bonding
B. Delley **423**

Call for Contributions **435**

Call for Contributions **437**

Issue No. 4, 1998

Special Issue: Symposium on Density Functional Theory and Applications (Part II of II)
Guest Editors: Weitao Yang and Mel Levy
Special Editor: Sam Trickey

Generation of Explicit Electron Correlation Functional by Means of Local Scaling Transformations
R. López-Boada, E. V. Ludeña, A. Karasiev, and R. Colle **439**

Fukutome Symmetry Classification of the Kohn–Sham Auxiliary One-Matrix and Its Associated State or Ensemble
B. Weiner and S. B. Trickey **451**

Rigorous Formulation of a Kohn and Sham Theory for States with Special Symmetries
A. K. Theophilou **461**

Exact Modified-Hartree–Fock Scheme Through Perturbation Expansion of Density Matrices
A. Holas **469**

Hartree–Fock Calculations in the Context of the Local-Scaling Transformation Version of Density Functional Theory. Applications to the Lithium and Beryllium Atoms
R. López-Boada and E. V. Ludeña **485**

General Hybrid Density Functional Theory
G. K.-L. Chan **497**

Atomic Kinetic- and Exchange-Energy Functionals by Means of Local-Scaling Transformations
R. López-Boada, V. Karasiev, E. V. Ludeña, and R. Colle **503**

Polynomial and Padé Representations for the Kinetic Component $T_c[\rho]$ of the Correlation Energy Density Functional
S. Liu, V. Karasiev, R. López-Boada, and F. De Proft **513**

A New Wigner-Like Correlation-Energy Functional from Coordinate Scaling Requirements
L. C. Wilson and S. Ivanov **523**

Virial Exchange–Correlation Energy Density in Hooke's Atom
K.-C. Lam, F. G. Cruz, and K. Burke **533**

Analysis of Density Functionals and Their Density Tails in H_2
P. W. Ayers, O. W. Day, Jr., and R. C. Morrison **541**

Density Functional Theory in Relation to X-Ray and Neutron Scattering Experiments
N. H. March **551**

A Modified Version of the Electron Localization Function (ELF)
P. Fuentealba **559**

Microscopic Functional Theory of Dielectrics
R. M. Martin and G. Ortiz **567**

Overcomplete Density Functional Description
J. K. Percus **573**

Virtual Space Level Shifting and Correlation Energies
J. Rey and A. Savin **581**

Kohn–Sham Description of Equilibria and Charge Transfer in Reactive Systems
R. F. Nalewajski **591**

Comparison of Density Functional and Hartree–Fock Average Local Ionization Energies on Molecular Surfaces
P. Politzer, F. Abu-Awwad, and J. S. Murray **607**

Prospects for a van der Waals Density Functional
J. F. Dobson **615**

A Theoretical Study of Rare-Gas Diatomic Molecules with the Generalized-Gradient Approximation to Density Functional Theory
D. C. Patton and M. R. Pederson **619**

Issue No. 5, 1998

Theoretical and Computational Developments

Nonadiabatic Molecular Theory and Its Application. II. Water Molecule
Y. Shigeta, Y. Ozaki, K. Kodama, H. Nagao, H. Kawabe, and K. Nishikawa **629**

Correlated Wave-Function Theory for Many-Center Many-Electron Problems
D. A. Shershakov and V. V. Nechaev **639**

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Semiempirical Configuration Interaction Calculations of XPS Shake-Up Satellites in $Ni(CO)_4$
J. Bustad and S. Lunell **649**

Ab Initio Study on the Internal Rotation of Five π-Conjugated Hydrocarbons at MP2 Level
X. Gong and H. Xiao **659**

Stability of Oxygen Anions and Hydrogen Abstraction from Methane on Reduced SnO_2 (110) Surface
Y. Yamaguchi, Y. Nagasawa, A. Murakami, and K. Tabata **669**

Complete Basis Set and Gaussian-2 Ab Initio Computational Studies of Planar Hückel and Möbius Aromatic Hydrogen Clusters
B. S. Jursic **679**

Book Review

The Quantum Challenge. By George Greenstein and Arthur G. Zajonc
E. Deumens **689**

Books Received **691**

Issue No. 6, 1998

Theoretical and Computational Developments

Relation Between BCS Hamiltonian and Ginzburg–Landau Equation
S. Aono **693**

Harmonic IR Spectra from Empirical Force Fields and Ab Initio Dipole-Moment Derivatives
D. Mathieu and P. Simonetti **705**

Dyson-Corrected Orbital Energies for the Perturbative Treatment of Electron Correlation
P. R. Surján and Á. Szabados **713**

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

$1/Z$ Expansion, Correlation Energy, and Shannon Entropy of Heavy Atoms in Nonrelativistic Limit
A. Grassi, G. M. Lombardo, N. H. March, and R. Pucci **721**

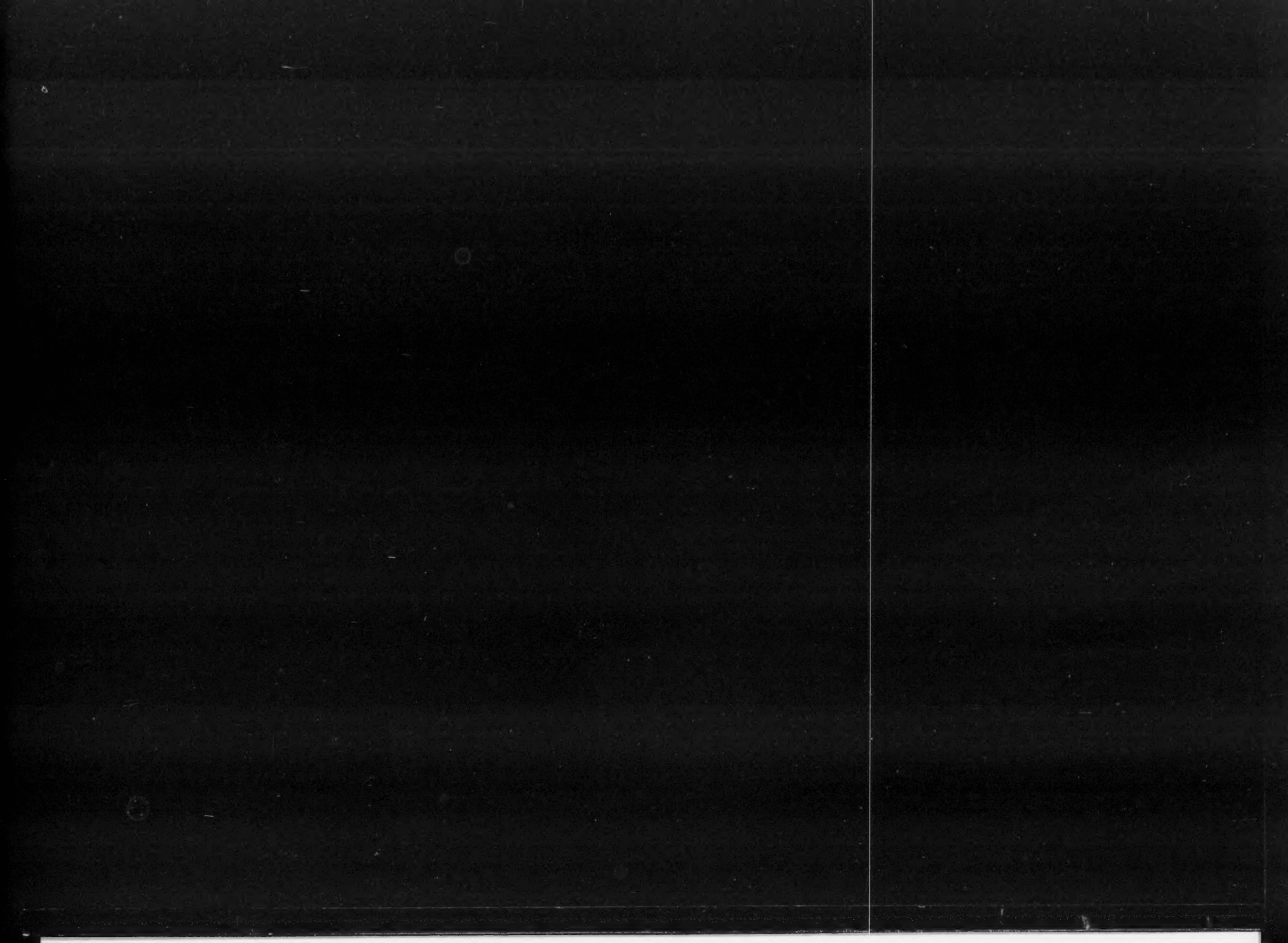
New Aspects in the Theory of π Electron Systems on the Basis of Quantum Statistical Considerations
M. C. Böhm, J. Schütt, and S. Philipp **727**

Molecular Structure, Dynamics, and Function of Biological Systems

Irreversible Inhibition of the HIV-1 Protease: A Theoretical Study
J. Mavri **753**

Volume Title Page **761**

Author Index **763**

Subject Index **767**

Volume Table of Contents ..... **I**